



IUCrData

ISSN 2414-3146

Received 7 December 2016

Accepted 9 December 2016

Edited by H. Stoeckli-Evans, University of Neuchâtel, Switzerland

Keywords: crystal structure; pyrazole; C—H... $\pi$  interactions.

CCDC reference: 1521904

Structural data: full structural data are available from iucrdata.iucr.org

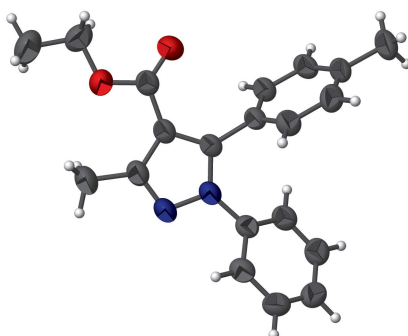
# Ethyl 3-methyl-1-phenyl-5-(*p*-tolyl)-1*H*-pyrazole-4-carboxylate

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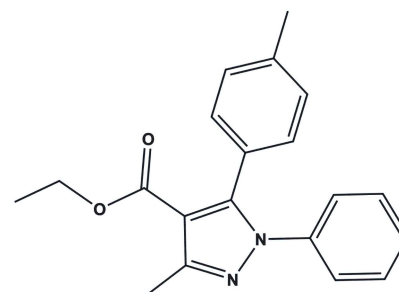
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In the title compound, C<sub>20</sub>H<sub>20</sub>N<sub>2</sub>O<sub>2</sub>, the pyrazole ring makes dihedral angles of 39.74 (8) and 60.35 (8)° with the phenyl and toluene rings, respectively. The dihedral angle between the phenyl and toluene rings is 62.01 (7)°.

## 3D view



## Chemical scheme



## Structure description

Pyrazoles are an important class of five-membered nitrogen heterocycles, which are very widely used as synthetic scaffolds for the construction of bioactive molecules (Ajay *et al.*, 2015). Apart from their synthetic utilities, pyrazole derivatives themselves exhibit a broad spectrum of biological activities (Farghaly *et al.*, 2012). As part of our studies in this area, we herein report on the crystal structure of the title compound.

The molecular structure of the title compound is shown in Fig. 1. The pyrazole ring (N1/N2/C1–C3) makes dihedral angles of 39.74 (8) and 60.35 (8)° with the phenyl (C8–C13) and the toluene (C14–C19) rings, respectively. The dihedral angle between the phenyl and toluene rings is 62.01 (7)°.

In the crystal, molecules are linked by C—H... $\pi$  interactions, forming chains propagating along the *a* axis (Table 1 and Fig. 2).

## Synthesis and crystallization

To a solution of (*E*)-ethyl 2-(4-methylbenzylidene)-3-oxobutanoate (0.01 mol), which was obtained by our earlier reported procedure (Naveen *et al.*, 2016), and phenylhydrazine hydrochloride (0.01 mol) in ethyl alcohol (20 ml), 3–4 drops of piperidine were

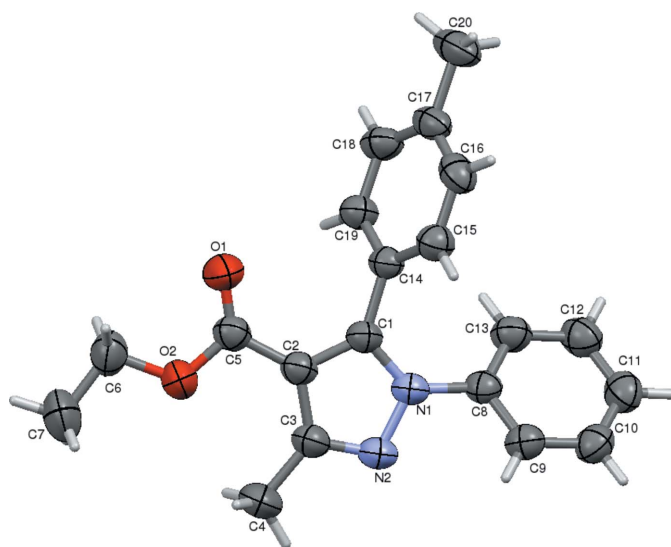


Figure 1

The molecular structure of the title compound, showing the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

added. The mixture was refluxed on a water bath for 3 h. The progress of the reaction was monitored by TLC. After completion, the mixture was poured into ice-cold water and the solid separated was filtered, and washed with ice-cold water to obtain the crude title product. The solid obtained was crystallized from methanol by slow evaporation giving pale-yellow rectangular-shaped crystals (90% yield; m.p. 358–359 K).

## Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

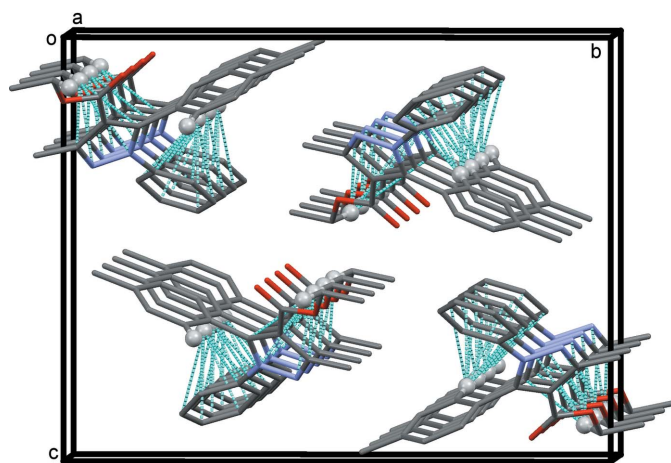


Figure 2

A view along the *a* axis of the crystal packing of the title compound. The C—H... $\pi$  interactions are shown as dashed lines (see Table 1) and, for clarity, only H atoms H6A and H19 (grey balls) have been included.

Table 1

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

*Cg*1 and *Cg*2 are the centroids of the N1/N2/C1–C3 and C8–C13 rings, respectively.

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C6—H6A... <i>Cg</i> 1 <sup>i</sup>	0.97	2.93	3.794 (2)	149
C19—H19... <i>Cg</i> 2 <sup>i</sup>	0.93	2.93	3.780 (2)	152

Symmetry code: (i)  $x - 1, y, z$ .

Table 2

Experimental details.

Crystal data	
Chemical formula	$\text{C}_{20}\text{H}_{20}\text{N}_2\text{O}_2$
$M_r$	320.38
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
<i>a</i> , <i>b</i> , <i>c</i> ( $\text{\AA}$ )	6.2796 (3), 18.9391 (9), 14.6430 (7)
$\beta$ ( $^\circ$ )	91.406 (2)
<i>V</i> ( $\text{\AA}^3$ )	1740.97 (14)
<i>Z</i>	4
Radiation type	Cu $K\alpha$
$\mu$ ( $\text{mm}^{-1}$ )	0.64
Crystal size (mm)	$0.29 \times 0.26 \times 0.24$
Data collection	
Diffractometer	Bruker X8 Proteum
Absorption correction	Multi-scan ( <i>SADABS</i> ; Bruker, 2013)
$T_{\min}$ , $T_{\max}$	0.837, 0.863
No. of measured, independent and observed [ $I > 2\sigma(I)$ ] reflections	13541, 2872, 2535
$R_{\text{int}}$	0.042
$(\sin \theta/\lambda)_{\text{max}}$ ( $\text{\AA}^{-1}$ )	0.585
Refinement	
$R[F^2 > 2\sigma(F^2)]$ , $wR(F^2)$ , <i>S</i>	0.045, 0.143, 1.06
No. of reflections	2872
No. of parameters	221
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$ , $\Delta\rho_{\text{min}}$ ( $\text{e \AA}^{-3}$ )	0.18, −0.13

Computer programs: *APEX2* and *SAINT* (Bruker, 2013), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *Mercury* (Macrae *et al.*, 2008) and *PLATON* (Spek, 2009).

## Acknowledgements

The authors are grateful to the Institution of Excellence, Vijnana Bhavana, University of Mysore, India, for providing the single-crystal X-ray diffractometer facility.

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## full crystallographic data

*IUCrData* (2016). **1**, x161972 [https://doi.org/10.1107/S2414314616019726]

Ethyl 3-methyl-1-phenyl-5-(*p*-tolyl)-1*H*-pyrazole-4-carboxylate

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Ethyl 3-methyl-1-phenyl-5-(*p*-tolyl)-1*H*-pyrazole-4-carboxylate*Crystal data*

$C_{20}H_{20}N_2O_2$	$F(000) = 680$
$M_r = 320.38$	$D_x = 1.222 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Cu $K\alpha$ radiation, $\lambda = 1.54178 \text{ \AA}$
Hall symbol: $-P 2_1/c$	Cell parameters from 2535 reflections
$a = 6.2796 (3) \text{ \AA}$	$\theta = 4.7\text{--}64.5^\circ$
$b = 18.9391 (9) \text{ \AA}$	$\mu = 0.64 \text{ mm}^{-1}$
$c = 14.6430 (7) \text{ \AA}$	$T = 296 \text{ K}$
$\beta = 91.406 (2)^\circ$	Block, yellow
$V = 1740.97 (14) \text{ \AA}^3$	$0.29 \times 0.26 \times 0.24 \text{ mm}$
$Z = 4$	

*Data collection*

Bruker X8 Proteum diffractometer	$T_{\min} = 0.837$ , $T_{\max} = 0.863$
Radiation source: Bruker MicroStar microfocus rotating anode	13541 measured reflections
Helios multilayer optics monochromator	2872 independent reflections
Detector resolution: $18.4 \text{ pixels mm}^{-1}$	2535 reflections with $I > 2\sigma(I)$
$\varphi$ and $\omega$ scans	$R_{\text{int}} = 0.042$
Absorption correction: multi-scan (SADABS; Bruker, 2013)	$\theta_{\max} = 64.5^\circ$ , $\theta_{\min} = 4.7^\circ$
	$h = -6 \rightarrow 7$
	$k = -21 \rightarrow 22$
	$l = -16 \rightarrow 17$

*Refinement*

Refinement on $F^2$	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.045$	$w = 1/[\sigma^2(F_o^2) + (0.0929P)^2 + 0.1486P]$
$wR(F^2) = 0.143$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{\max} < 0.001$
2872 reflections	$\Delta\rho_{\max} = 0.18 \text{ e \AA}^{-3}$
221 parameters	$\Delta\rho_{\min} = -0.13 \text{ e \AA}^{-3}$
0 restraints	Extinction correction: SHELXL97 (Sheldrick, 2008), $FC^* = KFC[1 + 0.001XFC^2\Lambda^3/\text{SIN}(2\Theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0058 (12)
Secondary atom site location: difference Fourier map	

*Special details*

**Geometry.** Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

**Refinement.** Refinement on  $F^2$  for ALL reflections except those flagged by the user for potential systematic errors.

Weighted R-factors  $wR$  and all goodnesses of fit  $S$  are based on  $F^2$ , conventional R-factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The observed criterion of  $F^2 > 2\sigma(F^2)$  is used only for calculating  $-R$ -factor-obs etc. and is not relevant to the choice of reflections for refinement. R-factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and R-factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	−0.0474 (2)	0.37329 (6)	0.57248 (10)	0.0816 (5)
O2	−0.06959 (18)	0.48057 (6)	0.63324 (9)	0.0694 (4)
N1	0.48074 (19)	0.36844 (6)	0.76439 (8)	0.0500 (4)
N2	0.4568 (2)	0.43678 (6)	0.79382 (9)	0.0585 (4)
C1	0.3333 (2)	0.35112 (7)	0.69887 (9)	0.0457 (4)
C2	0.2068 (2)	0.41063 (7)	0.68588 (10)	0.0497 (5)
C3	0.2920 (2)	0.46213 (8)	0.74707 (11)	0.0558 (5)
C4	0.2198 (3)	0.53571 (9)	0.76614 (16)	0.0826 (7)
C5	0.0209 (2)	0.41723 (8)	0.62416 (11)	0.0537 (5)
C6	−0.2603 (3)	0.49523 (10)	0.57961 (14)	0.0736 (6)
C7	−0.3193 (4)	0.56968 (13)	0.5990 (2)	0.1036 (10)
C8	0.6407 (2)	0.32691 (7)	0.81037 (9)	0.0486 (4)
C9	0.8308 (2)	0.35962 (8)	0.83481 (10)	0.0551 (5)
C10	0.9844 (3)	0.32222 (9)	0.88330 (11)	0.0623 (5)
C11	0.9497 (3)	0.25341 (9)	0.90858 (11)	0.0660 (6)
C12	0.7601 (3)	0.22121 (9)	0.88390 (12)	0.0673 (6)
C13	0.6040 (3)	0.25754 (8)	0.83511 (11)	0.0600 (5)
C14	0.3253 (2)	0.28043 (7)	0.65589 (9)	0.0459 (4)
C15	0.4968 (2)	0.25452 (8)	0.60870 (10)	0.0559 (5)
C16	0.4894 (3)	0.18672 (9)	0.57228 (11)	0.0627 (6)
C17	0.3139 (3)	0.14384 (8)	0.58204 (10)	0.0586 (5)
C18	0.1417 (3)	0.17121 (8)	0.62768 (11)	0.0600 (5)
C19	0.1455 (2)	0.23851 (8)	0.66403 (10)	0.0523 (5)
C20	0.3068 (4)	0.06983 (9)	0.54428 (14)	0.0861 (8)
H4A	0.07700	0.53470	0.78810	0.1240*
H4B	0.22330	0.56310	0.71100	0.1240*
H4C	0.31270	0.55670	0.81160	0.1240*
H6A	−0.37410	0.46360	0.59660	0.0880*
H6B	−0.23410	0.48910	0.51510	0.0880*
H7A	−0.34320	0.57510	0.66310	0.1550*
H7B	−0.44700	0.58160	0.56500	0.1550*
H7C	−0.20590	0.60040	0.58130	0.1550*
H9	0.85470	0.40640	0.81870	0.0660*
H10	1.11310	0.34390	0.89910	0.0750*
H11	1.05320	0.22880	0.94210	0.0790*
H12	0.73690	0.17440	0.90030	0.0810*
H13	0.47590	0.23560	0.81910	0.0720*
H15	0.61700	0.28240	0.60130	0.0670*
H16	0.60540	0.16990	0.54060	0.0750*

H18	0.02060	0.14360	0.63400	0.0720*
H19	0.02750	0.25580	0.69400	0.0630*
H20A	0.35410	0.03720	0.59070	0.1290*
H20B	0.39830	0.06660	0.49290	0.1290*
H20C	0.16350	0.05850	0.52520	0.1290*

*Atomic displacement parameters ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1	0.0878 (9)	0.0628 (8)	0.0926 (9)	0.0055 (6)	−0.0325 (7)	−0.0182 (6)
O2	0.0634 (7)	0.0566 (7)	0.0874 (8)	0.0107 (5)	−0.0141 (6)	−0.0085 (6)
N1	0.0539 (7)	0.0411 (6)	0.0547 (7)	−0.0030 (5)	−0.0019 (5)	−0.0072 (5)
N2	0.0651 (8)	0.0435 (7)	0.0665 (8)	−0.0021 (6)	−0.0072 (6)	−0.0127 (6)
C1	0.0480 (7)	0.0416 (7)	0.0476 (7)	−0.0049 (6)	0.0024 (6)	−0.0036 (6)
C2	0.0514 (8)	0.0425 (8)	0.0554 (8)	−0.0028 (6)	0.0036 (6)	−0.0040 (6)
C3	0.0599 (9)	0.0429 (8)	0.0646 (9)	−0.0014 (6)	0.0004 (7)	−0.0075 (7)
C4	0.0880 (13)	0.0513 (10)	0.1075 (15)	0.0084 (9)	−0.0172 (11)	−0.0246 (10)
C5	0.0553 (8)	0.0458 (8)	0.0602 (9)	−0.0034 (6)	0.0028 (7)	−0.0008 (7)
C6	0.0557 (9)	0.0732 (11)	0.0914 (13)	0.0050 (8)	−0.0087 (8)	0.0075 (9)
C7	0.0825 (14)	0.0865 (15)	0.141 (2)	0.0298 (12)	−0.0146 (14)	0.0011 (14)
C8	0.0544 (8)	0.0471 (8)	0.0443 (7)	−0.0018 (6)	0.0004 (6)	−0.0050 (6)
C9	0.0596 (9)	0.0526 (8)	0.0529 (8)	−0.0065 (7)	−0.0002 (7)	−0.0024 (6)
C10	0.0606 (9)	0.0696 (10)	0.0562 (9)	−0.0026 (7)	−0.0073 (7)	−0.0046 (7)
C11	0.0734 (11)	0.0681 (11)	0.0561 (9)	0.0117 (8)	−0.0079 (8)	−0.0008 (7)
C12	0.0848 (12)	0.0527 (9)	0.0642 (10)	0.0019 (8)	−0.0040 (8)	0.0054 (7)
C13	0.0653 (9)	0.0509 (9)	0.0635 (9)	−0.0079 (7)	−0.0024 (7)	−0.0001 (7)
C14	0.0527 (8)	0.0401 (7)	0.0447 (7)	−0.0015 (6)	−0.0015 (6)	−0.0028 (5)
C15	0.0555 (9)	0.0538 (9)	0.0586 (9)	−0.0014 (7)	0.0039 (7)	−0.0049 (7)
C16	0.0736 (10)	0.0595 (10)	0.0551 (9)	0.0184 (8)	0.0023 (7)	−0.0074 (7)
C17	0.0862 (11)	0.0392 (8)	0.0497 (8)	0.0059 (7)	−0.0135 (8)	−0.0011 (6)
C18	0.0748 (10)	0.0437 (8)	0.0610 (9)	−0.0127 (7)	−0.0065 (8)	0.0006 (7)
C19	0.0557 (8)	0.0460 (8)	0.0554 (8)	−0.0045 (6)	0.0028 (6)	−0.0041 (6)
C20	0.1353 (18)	0.0453 (9)	0.0765 (12)	0.0147 (10)	−0.0200 (12)	−0.0094 (8)

*Geometric parameters ( $\text{\AA}$ ,  $^\circ$ )*

O1—C5	1.197 (2)	C17—C18	1.386 (2)
O2—C5	1.3354 (19)	C17—C20	1.507 (2)
O2—C6	1.443 (2)	C18—C19	1.381 (2)
N1—N2	1.3736 (16)	C4—H4A	0.9600
N1—C1	1.3571 (17)	C4—H4B	0.9600
N1—C8	1.4310 (17)	C4—H4C	0.9600
N2—C3	1.3173 (19)	C6—H6A	0.9700
C1—C2	1.3893 (18)	C6—H6B	0.9700
C1—C14	1.4797 (19)	C7—H7A	0.9600
C2—C3	1.420 (2)	C7—H7B	0.9600
C2—C5	1.4640 (19)	C7—H7C	0.9600
C3—C4	1.494 (2)	C9—H9	0.9300

C6—C7	1.487 (3)	C10—H10	0.9300
C8—C9	1.3842 (18)	C11—H11	0.9300
C8—C13	1.384 (2)	C12—H12	0.9300
C9—C10	1.379 (2)	C13—H13	0.9300
C10—C11	1.374 (2)	C15—H15	0.9300
C11—C12	1.378 (3)	C16—H16	0.9300
C12—C13	1.382 (3)	C18—H18	0.9300
C14—C15	1.3837 (19)	C19—H19	0.9300
C14—C19	1.3878 (19)	C20—H20A	0.9600
C15—C16	1.391 (2)	C20—H20B	0.9600
C16—C17	1.379 (3)	C20—H20C	0.9600
C5—O2—C6	117.92 (13)	H4A—C4—H4B	109.00
N2—N1—C1	111.81 (11)	H4A—C4—H4C	109.00
N2—N1—C8	116.83 (11)	H4B—C4—H4C	109.00
C1—N1—C8	131.19 (11)	O2—C6—H6A	110.00
N1—N2—C3	105.73 (12)	O2—C6—H6B	110.00
N1—C1—C2	106.18 (12)	C7—C6—H6A	110.00
N1—C1—C14	122.33 (12)	C7—C6—H6B	110.00
C2—C1—C14	131.49 (12)	H6A—C6—H6B	109.00
C1—C2—C3	105.40 (12)	C6—C7—H7A	110.00
C1—C2—C5	126.75 (13)	C6—C7—H7B	109.00
C3—C2—C5	127.82 (12)	C6—C7—H7C	109.00
N2—C3—C2	110.89 (13)	H7A—C7—H7B	109.00
N2—C3—C4	118.75 (14)	H7A—C7—H7C	110.00
C2—C3—C4	130.33 (14)	H7B—C7—H7C	109.00
O1—C5—O2	122.73 (14)	C8—C9—H9	120.00
O1—C5—C2	126.78 (14)	C10—C9—H9	120.00
O2—C5—C2	110.49 (13)	C9—C10—H10	120.00
O2—C6—C7	106.61 (17)	C11—C10—H10	120.00
N1—C8—C9	117.82 (12)	C10—C11—H11	120.00
N1—C8—C13	121.71 (13)	C12—C11—H11	120.00
C9—C8—C13	120.36 (13)	C11—C12—H12	120.00
C8—C9—C10	119.41 (14)	C13—C12—H12	120.00
C9—C10—C11	120.82 (16)	C8—C13—H13	120.00
C10—C11—C12	119.40 (16)	C12—C13—H13	120.00
C11—C12—C13	120.83 (16)	C14—C15—H15	120.00
C8—C13—C12	119.17 (16)	C16—C15—H15	120.00
C1—C14—C15	120.97 (12)	C15—C16—H16	119.00
C1—C14—C19	120.02 (12)	C17—C16—H16	119.00
C15—C14—C19	119.00 (13)	C17—C18—H18	119.00
C14—C15—C16	119.99 (13)	C19—C18—H18	119.00
C15—C16—C17	121.55 (16)	C14—C19—H19	120.00
C16—C17—C18	117.69 (15)	C18—C19—H19	120.00
C16—C17—C20	121.75 (17)	C17—C20—H20A	109.00
C18—C17—C20	120.56 (17)	C17—C20—H20B	110.00
C17—C18—C19	121.65 (15)	C17—C20—H20C	109.00
C14—C19—C18	120.08 (13)	H20A—C20—H20B	109.00

C3—C4—H4A	110.00	H20A—C20—H20C	109.00
C3—C4—H4B	109.00	H20B—C20—H20C	109.00
C3—C4—H4C	109.00		
C6—O2—C5—O1	1.5 (2)	C5—C2—C3—N2	178.10 (14)
C6—O2—C5—C2	−177.83 (13)	C5—C2—C3—C4	0.1 (3)
C5—O2—C6—C7	−176.98 (16)	C1—C2—C5—O1	−3.0 (3)
C1—N1—N2—C3	0.62 (16)	C1—C2—C5—O2	176.28 (13)
C8—N1—N2—C3	−175.18 (12)	C3—C2—C5—O1	179.34 (16)
N2—N1—C1—C2	−0.61 (15)	C3—C2—C5—O2	−1.4 (2)
N2—N1—C1—C14	179.93 (12)	N1—C8—C9—C10	176.73 (13)
C8—N1—C1—C2	174.41 (13)	C13—C8—C9—C10	0.7 (2)
C8—N1—C1—C14	−5.1 (2)	N1—C8—C13—C12	−176.41 (14)
N2—N1—C8—C9	−39.04 (17)	C9—C8—C13—C12	−0.5 (2)
N2—N1—C8—C13	136.99 (14)	C8—C9—C10—C11	−0.9 (2)
C1—N1—C8—C9	146.15 (14)	C9—C10—C11—C12	1.0 (3)
C1—N1—C8—C13	−37.8 (2)	C10—C11—C12—C13	−0.8 (3)
N1—N2—C3—C2	−0.38 (16)	C11—C12—C13—C8	0.6 (3)
N1—N2—C3—C4	177.88 (14)	C1—C14—C15—C16	177.18 (13)
N1—C1—C2—C3	0.35 (15)	C19—C14—C15—C16	−1.6 (2)
N1—C1—C2—C5	−177.75 (13)	C1—C14—C19—C18	−176.92 (13)
C14—C1—C2—C3	179.74 (14)	C15—C14—C19—C18	1.9 (2)
C14—C1—C2—C5	1.6 (2)	C14—C15—C16—C17	−0.1 (2)
N1—C1—C14—C15	−60.00 (19)	C15—C16—C17—C18	1.6 (2)
N1—C1—C14—C19	118.79 (15)	C15—C16—C17—C20	−178.80 (16)
C2—C1—C14—C15	120.70 (17)	C16—C17—C18—C19	−1.3 (2)
C2—C1—C14—C19	−60.5 (2)	C20—C17—C18—C19	179.07 (16)
C1—C2—C3—N2	0.03 (16)	C17—C18—C19—C14	−0.4 (2)
C1—C2—C3—C4	−177.97 (16)		

### Hydrogen-bond geometry ( $\text{\AA}$ , $^\circ$ )

Cg1 and Cg2 are the centroids of the N1/N2/C1–C3 and C8–C13 rings, respectively.

$D\cdots H\cdots A$	$D\cdots H$	$H\cdots A$	$D\cdots A$	$D\cdots H\cdots A$
C6—H6A $\cdots$ Cg1 <sup>i</sup>	0.97	2.93	3.794 (2)	149
C19—H19 $\cdots$ Cg2 <sup>i</sup>	0.93	2.93	3.780 (2)	152

Symmetry code: (i)  $x-1, y, z$ .